Journal of Technology and Science Education

A FREE ACCESSIBLE INDIVIDUAL-BASED SIMULATOR ENABLING VIRTUAL EXPERIMENTS ON SOIL ORGANIC MATTER PROCESSES IN CLASSROOM

Anna Gras[1], Juan Carlos Cañadas[2], Marta Ginovart[3]

1 Department of Agri-Food Engineering and Biotechnology, Technical University of Catalonia, Edifici D4, Esteve Terradas 8, 08860 Castelldefels (Barcelona), Spain
2 Department of Physics and Nuclear Engineering, Technical University of Catalonia, ETSEIAT, Edifici TR5, Colom 11, 08222 Terrassa (Barcelona), Spain
3 Department of Applied Mathematics III, Technical University of Catalonia, Edifici D4, Esteve Terradas 8, 08860 Castelldefels (Barcelona), Spain

anna.gras@upc.edu, juan.carlos.canadas@nobel.upc.edu, marta.ginovart@upc.edu

Received February 2013
Accepted July 2013

Abstract

This work addresses and aims to fulfil a very clear need in teaching biosystem engineering. When introducing students to the complexity of soil processes, one of the frustrations that teachers often experience is the impossibility to demonstrate practically, in the lab, some of the concepts and processes discussed in class. Either the experiments take far longer than a typical laboratory session or they require access to specific equipment. To deal with this situation, it would be ideal for students to be able to do virtual experiments. The purpose of this work is to display the individual-based simulation model INDISIM-SOM, available free from a website, and to show how it can be used in experiments or as a teaching-learning instrument in the classroom. The computational model has been designed specifically for the study of soil organic matter and is based mainly on the activity conducted by two different prototypes of microorganisms. One option of using INDISIM-SOM is as a way to introduce the individual-based model as a methodology to improve understanding of the agents involved in soil microbial system and their processes. Another option is to develop the ability to work with simulators by connecting concepts and helping students in the development of modelling competence. Virtual experiments were carried out as an example of what may be expected from using the INDISIM-SOM web simulator. Temporal evolutions of five virtual soils with different organic C content and proportional content in organic N, easily hidrolyzable N, nitrate and ammonia were generated and discussed.

Keywords *– biosystems engineering education, computational model, individual-based simulations, virtual experiment, soil organic matter processes*

----

1 INTRODUCTION

Modelling is a necessary tool to represent, analyze and discuss aspects or ideas related to biological systems from a general perspective (Murray, 1990). With this in mind, teaching soil science based on the development of models is widely accepted in the academic community (Justi, 2006, Faraco & Gabriele, 2007; Bravo, van Joolingen & de Jong, 2009; Thompson & Reimann, 2010; and so on). Continuous mathematical modelling based on continuous and/or derivable functions, differential equations, methods for optimization, fittings of curves and statistical modelling are the methodologies usually studied in mathematics courses, both in high school and during the early years of university studies in the fields of science and technology. Most university curricula address the acquisition of competence in the modelling process, ensuring that students understand how a system functions and acquire the ability to develop a model in their subject area. In this sense, the availability of simulators and their use contributes to autonomous learning by students.

In the nineties, a new approach to modelling complex systems, referred to as individual-based modelling (IBM), began to emerge, characterized by both a philosophy and perspective that were different from the continuous models predominantly used until then. This approach is also known as biological agent-based models. In IBM models, the individuals that make up the system are treated as autonomous and discrete entities (Grimm & Railsback, 2005; Grimm, Berger, Bastiansen, Eliassen, Ginot, Giske, et al., 2006; Grimm, Berger, DeAngelis, Polhill, Giske & Railsback, 2010). The models focus on the characterization of these entities by means of rules of behavior, which allow the elements to interact with one another and with the environment in which they are evolving. These computational models require distinct simplifications from those assumed by continuous models, and they are a good modelling alternative to deal with specific aspects related to biosystems (Grimm & Railsback, 2005).

Multidisciplinary courses are being developed at a number of colleges and universities that highlight the use of soils in agriculture and the sustainable or unsustainable uses of natural resources. The content of the courses is usually complex, as it includes concepts from such varied disciplines as soil science, geology, chemistry, physics and microbiology. The learning goals for these courses include developing skills in the critical analysis of complex soil systems. In an attempt to address these issues, activities that focus on the connections existing between the different elements that make up the soil system and the intricate processes evolving in it are especially beneficial (Jacobson, Militello & Baveye, 2009). One way to deal with all of these items is by using modelling and simulation as tools for teaching and learning.

In certain contexts, computational models offer the potential to reduce, or even replace, some experimental assays required when exploring new substrates and/or process options. Various researchers have postulated that simulation models are a new kind of experimental system (Peck, 2004). The present study is based on the perspective that a mechanistic and scale-dependent description of microbial activity, with detailed formulation of microbial biomasses and their relationships with organic and inorganic substrates, is essential when dealing with the dynamics of C and N in soil organic matter (SOM). Nevertheless, to describe the microbial activity, and not just the amount of microbial biomass, we need to explain transient fluxes as a reaction to environmental changes. In order to provide the approach needed for diverse scenarios under different conditions, one way to proceed is by using IBMs (or agent-based models), from which macroscopic patterns can be inferred (Hellweger & Bucci, 2009).

This work addresses and seeks to fulfil a very clear need in teaching. When introducing students to the enormous complexity of soil processes, one of the frustrations that teachers often experience is their inability to demonstrate many of the concepts or processes discussed in class practically, in a laboratory setting. Either the experiments take far longer than a typical laboratory session or they require access to equipment that is not generally found in a typical undergraduate teaching lab. In light of this situation, it would be ideal for the students to be able to conduct virtual experiments with a web-based simulation tool that would provide a reasonably realistic depiction of what really happens in soil.

INDISIM-SOM, an IBM that deals with the dynamics and evolution of C and N in the organic matter in soil by controlling a microbial soil population and a set of diverse organic and inorganic compounds, has been used successfully in research (Ginovart, Gras & López, 2005; Gras, Ginovart, Portell & Baveye, 2010b; Gras, Ginovart, Valls & Baveye 2011). Moreover, we are convinced that INDISIM-SOM is a good instrument for the study of SOM modelling, contributing to the acquisition of modelling competence at different academic levels. A website was designed and developed to make the INDISIM-SOM simulator accessible to the scientific community (Gras, Cañadas & Ginovart, 2010a), which also makes it available for use as a teaching and learning tool.

The objectives of the present study are:

- To present the INDISIM-SOM model according to the recent update Overview – Design concepts – Details protocol (ODD protocol) established by Grimm and co-authors, in order to standardize its general description, making it more rigorous, understandable and complete (Grimm et al., 2006, 2010). At the same time, the various stages of the modelling process will be reviewed in detail, illustrating how learners should proceed with this type of modelling.
- To show how this simulator, implemented on a free access website, can be used to perform virtual experiments related to SOM mineralization and nitrification processes, further advance the skills associated with the simulation model and illustrate some practical exercises to be carried out in the classroom with different scenarios where the C and N soil determinations have different values.

The implementation of classroom activities using the INDISIM-SOM simulator with a group of second-year students studying Biosystems Engineering at the Universitat Politècnica de Catalunya will be discussed in this context. Two questionnaires were prepared to assess the students' knowledge of microbial activity in SOM before and after these activities, in order to compare and assess the acquisition of additional concepts at the end of the proposed activities (https://aneto.upc.es/simulacio2/Pre_test.pdf).

2 MODELLING, EDUCATION AND SOIL SCIENCE

In biology, there are several areas of knowledge in which the use of IBMs is constantly expanding (Ginovart, Prats, Portell & Silbert 2011; Gras et al., 2010b, 2011; Grimm et al., 2010; Hellweger & Bucci, 2009; McLane, Semeniuk, McDermid & Marceau, 2011; Prats, Ferrer, Gras & Ginovart, 2010; etc.). Most of the fields of biology in which they are being applied are concerned with the study of population dynamics, such as predator-prey marine populations, agricultural systems and ecology, among others. In recent years, a large number of specialized journals in different areas have published studies in which IBMs are used, and they have recently been established as a suitable tool for describing and working with complex systems made up of autonomous entities. Furthermore, they are increasingly being used in teaching and learning (Levy & Wilensky, 2011; Railsback & Grimm, 2011; Wilensky & Reisman, 2006). This type of computational model has an advantage over other methodologies in that it facilitates virtual experimentation and management of systems, permitting the observation and recurring analysis of the set of simulations resulting from the implementation of the IBM in a suitable framework, while changing individual parameters or starting conditions of the system (Peck, 2004).

Unlike continuous models, IBMs are conceptually easy to understand and do not require mastery of advanced mathematical theories. For this reason, it would seem that they might be a useful tool from an educational perspective, as they can be utilized by a wide sector of users. In the field of biology, the use of IBMs offers a great opportunity for working at different stages involved in a modelling process. Some concepts linked to competence, cooperation, adaptation, diversity, individuality and variability may be easier to explain and work with using IBMs than with other mathematical modelling methods.

2.1 Soil Science And Education

The world is becoming more and more urbanized, with a large number of people living and working in or around cities, whose only connection with nature is for leisure. This, along with the increasing consumption of processed foods, has led to a lack of knowledge about agriculture and the reasonable use of natural resources. Many of these people may never consider that soil can be degraded or that it is essential for the intensive agriculture necessary to support their urban lifestyles (Jacobson et al., 2009).

A very interesting review of soil biogeochemical models, with an extensive comparison of mathematical approaches to soil carbon (C) and nitrogen (N) cycling, was provided by Manzoni and Porporato (Manzoni & Porporato, 2009). Some key processes in C and N cycling in soils are the decomposition and mineralization of organic matter, N immobilization and nitrification. In the majority of models developed in recent decades, these processes are analyzed according to the common framework of substrate-decomposer stoichiometry, focusing on the role of microbial biomass as a SOM mineralization and N cycling agent. Most new models are improvements on earlier ones, leading to many similar model structures and formulations. While this has generally produced more robust and effective models, it may have also delayed significant theoretical advances and shifted attention away from some important questions that have therefore remained unexplored. For example, few models explicitly describe the spatial dynamics of water, organic matter and nutrients at microscopic scales. Manzoni and Porporato conclude their review by discussing some of the theoretical gaps that have been identified and suggest ways in which they could be addressed by future modelling efforts (Manzoni & Porporato, 2009). The model presented here should be considered along these lines. This contribution has been made in order to prepare future scientists, targeting different levels in the education of future generations. It is from academic activity that new perspectives can be delineated in the study of such a complex system as SOM.

IBMs are generally built upon more realistic assumptions than continuous models, in the sense that they are based on biological events. A further effort is certainly necessary to expand the use of IBMs in soil research. Throughout the past few decades, numerous models of the C and N cycle have been developed, especially for agricultural and ecological purposes. Some were aimed at predicting long-term SOM changes, whereas others were created to reproduce short-term evolutions, so as to determine the environmental impact of different soil

management systems and land use strategies. Most of the models are structurally similar because they are based on a given number of SOM compartments with different turnover rates. Furthermore, the microbial biomass is usually handled as an active pool of SOM, but not as an ensemble of individual organisms with their own activity, capabilities and growth. In this sense, IBMs offer the possibility of considering individuals as entities defined by their own biological or physical characteristics and activities. This modelling methodology offers insight into the mechanisms and interactions of the constituent entities of a complex system, the macroscopic behavior of which can be expressed in terms of a physiological process. Nevertheless, successful applications of IBMs are highly dependent upon the biological data available for these individual entities, microorganisms and substrates.

2.2 IBMs And Education

At present, IBMs are not included in the teaching material used to develop competence in modelling, which is considered to be very important for the achievement of a complete background in science. There are many factors that may explain this absence, such as the non-existence of standards for procedures in the formulation and programming of IBMs and lack of experience in the presentation and communication of this kind of model. This has served to limit acceptance of these models in the academic world. It should be added that since IBMs are computational models, they must be implemented in programming code and executed in an appropriate computing framework to analyze the outcomes. It seems this is also one of the reasons why the potential of this type of modelling has not been fully exploited and developed in the academic world. Access to computerized frameworks for working with IBMs would greatly facilitate this task and contribute to the efficient use of simulators. Therefore, we are convinced that any help that can be offered to explore the possibilities of IBMs is crucial and will be decisive in achieving their widespread acceptance in teaching (Ginovart, Portell, Ferrer-Closas & Blanco, 2012).

Continuous models are easy to represent, as they employ universal mathematical language, mathematical and statistical symbols, and they have formed part of most people's academic training since the beginning. In contrast, IBMs have characteristics and essential designs that cannot be described by means of equations and parameters with a synthetic formulation. IBMs do not have a globally accepted common language for their communication, and are usually too broad to be completely described in a single informative or scientific publication. Many of the descriptions of IBMs that have been published are difficult to read, incomplete and ambiguous, and so remain rather inaccessible (Grimm et al., 2006). Solving the problem of how to communicate IBMs may increase their scientific credibility. There are two main interrelated factors that determine the way in which IBMs are presented: i) until a few years ago, with no protocol to follow for its description, each IBM was explained according to the criteria and preferences of the authors, who generally belonged to diverse areas of research (ecology, mathematics, engineering, botany, physics, chemistry, microbiology, veterinary studies, etc.); ii) without the option of having a complete computational code for the IBM, the description was mainly verbal, with a great deal of text and no clear indication of equations, rules or schemes, and without any pre-established order or consensus on how to transmit the information contained in the computational model. Very often a thorough, careful reading of everything that the simulator is able to control and reproduce is excessive, and an inefficient means of obtaining relevant knowledge about the model, general structure and fundamental features. General considerations are often mixed with descriptions of processes, justifications of the formulas used and previous hypotheses.

A partial solution to these problems would be to reach an agreement in the scientific community regarding the means of presenting and communicating IBMs, unifying the criteria for these descriptions. With this in mind, in 2006, Grimm and a group of 26 modellers with experience in this modelling methodology produced a protocol which identified the blocks and elements that make up its structure, and which has recently been revised and updated (Grimm et al., 2006, 2010).

3 THE TOOL

The INDISIM-SOM model was developed to study the dynamics of SOM for different mineral soils under controlled conditions.

The simulator INDISIM-SOM was written in Fortran and compiled by g95, which is based on the free software GNU Compiler Collection (GCC). A version of INDISIM-SOM is available on the website https://aneto.upc.es/simulacio2/hoja-portada.html (Gras et al., 2010a). The operating systems Mandriva Linux

(in a server computer) and CentOS 5.5, with a free cluster management system (in a computer cluster), were used. The server uses Cascading Style Sheets (CSS) to describe the presentation (the look and formatting) of documents written in Hypertext Mark-up Language (HTML) in order to to construct the web pages. Calculations are made using the simulation program in Fortran, which is located in the computer cluster. Java language is used on the system application server. JfreeChart is the open-source framework for the programming language Java that makes it possible to read the data and create the graphic representations. Networking between the server and the cluster is carried out by means of the Hypertext Preprocessor (PHP), designed for producing dynamic web pages. This code is embedded in the HTML source document and interpreted by a web server computer. Finally, Samba (free networking standard protocol software), a set of tools to share resources on a TCP/IP network, was also used. All programs used in the construction of INDISIM-SOM web are released under a General Public License.

This website is composed of the following: i) a brief theoretical introduction to the general model, ii) a demonstration of the simulator, with graphical outputs for certain variables related to C and N (Demo option) and iii) access to an executable version of the simulator that allows changes in the values of some parameters (Log in option).

The INDISIM-SOM input data offered on the website to be modified jointly with the graphical outputs make it possible to configure different simulations and to study the soil system behavior through the simulator. The parameters that can be changed before starting the simulation are associated with: i) soil analyses, mainly the analytical determinations related to C and N content, ii) fractionation constants, which relate the experimental determination to SOM compartments in the model, and iii) microbial constants. The simulator is not appropriate for use with all soils or sets of values, so it is necessary to specify the ranges of the model parameters in order for the simulator to operate as expected. In this sense, it is necessary to take into account the fact that this simulator was parameterized and calibrated to reproduce C and N dynamics in soils incubated under fixed external conditions (Ginovart et al., 2005; Gras et al., 2010b, 2011), and therefore the temperature and the moisture should be more or less constant. The simulator works for mineral soils when the amounts of C and organic N are set within specific ranges of values.

4 DESCRIPTION OF THE MODEL

IBMs have been criticized as being so poorly documented that the models cannot be evaluated or compared efficiently. These criticisms prompted the creation of the ODD (Overview, Design concepts, Details) protocol, which attempted to create a generic format and a standard structure to explain all IBMs (Grimm et al., 2006). The primary purpose of ODD was to make the writing and reading of model descriptions easier and more efficient. Apart from the expected practical benefits of providing a systematic documentation of models, the ODD protocol helps promote a more rigorous formulation of models, as it provides a comprehensive checklist that covers virtually all of the key features that can characterize a model and that need to be described.

Descriptions of different parts of INDISIM-SOM, according to the diverse aims of the studies carried out so far with this simulation model, can be found in some previously published papers (Ginovart et al., 2005; Gras et al., 2010b, 2011). Nevertheless, a description of this model following the revised and updated OOD protocol (Grim et al., 2010) has not yet been provided. With the presentation of INDISIM-SOM under the structure of this protocol, a more self-contained, autonomous and complete idea of the model will be provided, which is a fundamental prerequisite to enable the efficient use of this simulator via the free access website developed to interact with it. In addition, if our objective is to extend this kind of modelling to learners, this is the manner in which this kind of modelling must be presented in an educational context.

4.1 Purpose

The aim of INDISIM-SOM is to simulate the mineralization of C and N and the nitrification and humification processes of soil organic matter, taking into account the activity of the microorganisms as the main agents which drive these processes.

4.2 Entities, State Variables And Scales

IBM considers individuals and their physical environment.

The individuals, microorganisms of two prototypes (decomposers with heterotrophic metabolism and nitrifiers with autotrophic metabolism), are characterised by a set of state variables. These individual variables take into account the microbial prototype, spatial position, biomass, mass required to start the reproduction, minimum mass to dye, and internal storage of organic C and N substrates. The biomass composition of each microbial class is defined by the C to N ratio, a_i, which is 7 for heterotrophs (i = 1) and 5 for nitrifiers (i = 2).

The physical environment is characterized by: (i) the coexistence of three physical phases, gas, liquid and solid, where the different soil fractions are located, and (ii) the composition of the different organic matter substrates and inorganic components.

The environment state variables are provided on a discrete two-dimensional grid, where each spatial cell is characterized by its Cartesian coordinates (x,y). In each spatial cell, the variables under control are the number of individuals of each prototype and the quantity of organic and mineral substrates contained in each fraction of the soil:

- The solid fraction consists of the polymeric substrates C_P and CN_P, the resistant compounds C_R and CN_H, and adsorbed ammonia, all of which have a fixed position in the space.
- The liquid fraction contains the soluble compounds: labile substrates, i.e., labile C (C_L) and labile N (CN_L), nitrate (N_{NO3}), soluble ammonia (N_{NH4}), oxygen (O_2), and carbon dioxide (C_{CO2}).
- The gas fraction corresponds to the soil atmosphere, and is composed of oxygen and carbon dioxide.

Processes are modelled discretely, and events take place at finite time steps. The time step is set as 30 minutes.

The simulation represents 1g of a homogenized soil system stored in a container for 90 days. The space is modelled as a two-dimensional lattice, composed of 30×30 spatial cells. Therefore, if we assume a bulk density of 1.3 g cm^{-3}, the characteristic length of the domain is 0.916 cm. The bulk density of soil is inversely related to its porosity, so the assumed porosity of this bulk density is nearly 51% of the volume. According to the simulated humidity conditions, this porosity is filled with 13-18% water (w/s) and 33-38% air (a/s), depending on the soil texture.

The obvious disadvantage of modelling populations on an individual basis is that it takes too much computation time to simulate realistic numbers for most populations, especially if the individual behavior is rather complex, as is the case in many applied models, such as INDISIM-SOM. In this kind of approach, the concept of "super-individuals" is presented as a convenient solution (Scheffer, Baveco, DeAngelis, Rose & van Nes, 1995). Due to the large number of microorganisms in 1 g of soil and the difference in magnitude between the number of microorganisms belonging to the two prototypes considered in the population (decomposers and nitrifiers), it is necessary to divide individuals into groups or classes. Therefore, an additional feature of each individual model is the number of microorganisms that constitute a ‘super-individual’. Thus, the resulting "super-individuals" are nothing other than 'generalized individuals'. This is a strategy used to model large populations on an individual basis (Scheffer et al., 1995). In this way, the essence of the individual is not lost, because when a simulation is performed, it is considered that many individuals (one super-individual) with similar characteristics are acting in the same way at one time step, in order to avoid computational problems. The number of super-individuals modelled and acting at each time step can be greater than 5×10^3.

4.3 Process Overview And Scheduling

The process that follows the simulation has been widely described and discussed in previous works involving the simulator INDISIM and its different versions, and it is beyond the scope of this text to detail all the general features it offers. We may refer the interested reader to previous papers (for example, Ginovart et al., 2011; Gras et al., 2010a, 2010b, 2011; Prats et al., 2010). Only a few specific aspects will be mentioned to focus directly on the later use of the simulator INDISIM-SOM.

Individual microbial actions and mass transfer processes take place at each time step of the evolution. Each individual carries out its actions: uptake, metabolism, death and lyses and reproduction. They act sequentially, but the order in which they act changes randomly at each time step. Individual actions alter only the spatial cell in which they occur. The changes in the spatial cell due to individual processes are updated as the individual action occurs. The mass transfer processes that take place in each spatial cell are the hydrolysis of humic and polymeric substrates into labile substrates, adsorption and desorption of ammonia, oxygen diffusion from the

atmosphere to the soil solution, and the output of CO_2 and substrate diffusion. The general characteristics of the system are updated only after all spatial cell processes have been performed. At the end of each time step, outcome data are stored as output data for further analysis.

4.4 Design Concepts

4.4.1 Emergence

Population dynamics show that the increase in the nitrifier subpopulation follows an increase of heterotrophic activity, according to the properties and characteristics of the environment in which it is evolving (Silva, Jorgensen, Holub & Gonsoulin, 2005). This succession of subpopulations is not modelled explicitly, rather it emerges as a consequence of (i) the higher labile C availability in the early steps, promoting heterotrophic metabolism and microbial growth for the population with the consequence of ammonia immobilization and a large reduction in oxygen availability, and (ii) the large quantities of ammonia required for nitrifiers as an energy source; therefore, the competence of that substrate implies that the nitrifiers do not start to grow until heterotrophic population decay has occurred.

Some results or outputs of the simulator are identified as emerging from the adaptive traits, or behaviors, of individuals. For instance, due to the absence of labile compounds (kinetic constants equal to 0), the heterotrophic population cannot survive, so the nitrifier individuals will lose population until they disappear, because the ammonia consumed is not restored from the mineralization of organic N. But if the ammonia in soil solution is 0 (adsorption constant of ammonia equal to 1), then the heterotrophics will grow using organic N as an N source, but nitrifiers will only survive if there is degradation of microbial biomass. Accordingly, the heterotrophic population is positioned below the nitrifier on the food web chain, since it has greater metabolic diversity, which allows for better survival rates.

4.4.2 Adaptation

In contrast to nitrifiers, the metabolic diversity of heterotrophics provides them with greater adaptability to the local medium composition; they have different sources of N, organic N (CN_L), ammonia (N_{NH4}), nitrate (N_{NO3}), C, and labile C (C_L), as well as labile N (CN_L), as defined by its C to N ratio.

4.4.3 Objectives

The heterotrophic individuals require diverse sources of C and N in order to be viable. For maintenance, the use of one substrate or another simply follows the established preference, C_L, CN_L and its biomass. The individuals do not make decisions; it is merely a matter of substrate availability in the spatial cell. Nitrifiers proceed in the same way, using N_{NH4} as the first option, and its biomass as the second. For biomass synthesis, heterotrophics can use only C_L as a C and energy source, but they can use three N sources, N_L, N_{NH4}, and N_{NO3}, in this order of preference.

4.4.4 Sensitivity

The individuals are sensitive to their environmental conditions, particularly to nutrient availability and aerobic conditions.

4.4.5 Interaction

The presence of several individuals in the same local environment permits interaction among them, due to: (i) local intra-specific and inter-specific competition for substrates and oxygen among individuals, and (ii) the changes in local environment caused by microbial activity (i.e., hydrolysis, microbial lysis and the subsequent release of ammonia and polymeric or humic substrates into the medium).

4.4.6 Stochasticity

Randomness is introduced in two ways. Firstly, we consider the heterogeneity among individuals. Some of their characteristics are assigned by random variables with specific distributions of probability. In addition, randomness is also considered in the updating of some individual actions. Secondly, uncertainty and variability are introduced into the mass transfer process in the medium (hydrolysis reactions). Both of these are

introduced as Gaussian noise on the mean or expected values. The released location of each individual is chosen randomly.

4.4.7 Observation

The output data are collected at the end of each time step. The output variables shown by the web simulator belong to the system, so they are the result of the sum of all individualities and are converted into commonly used experimental determinations. The output graphical representations on the web are organized into those variables directly representative of C and N mineralization and nitrification, such as net CO_2 production, mineral N, easily hydrolyzable N, ammonia and nitrate, and those linked to soil microbial composition and oxygen, such as the ratio of C_{MIC} to C_{ORG}, number of heterotrophic individuals, number of nitrifiers, C to N microbial ratio and % of oxygen (Gras el al., 2010a).

However, it is also feasible to obtain other microbial parameters to characterize the microbial population, such as mortality, lysis and maximum growth rate.

4.5 Initialization

The simulations begin with the reading of input parameters in order to set the initial configuration of the system. These parameters can be sorted into: (i) soil analyses or composition, (ii) soil parameters (i.e. fractioning constants and kinetic constants, and (iii) microbial parameters (death probability and maintenance energy). The calibration of the model and the sensitivity analyses of biotic (microbial) and abiotic (soil) parameters are described in the studies by Gras et al. (2010b and 2011). Table 1 shows the parameters that may be modified in the web simulator, and the range of values in which the simulations make sense.

4.6 Submodels

Submodels account for the actions that take place in the local environment and the rules of behavior followed by the microorganisms.

4.6.1 Modelling The Space

The phenomena taken into account by the current spatial model are sufficient to cover the most important spatial effects in a soil sample incubated at constant temperature, periodically aerated, and with moisture close to field capacity. The phenomena considered are:

- Hydrolysis reactions: from polymerized and humic compounds to labile substrates. The kinetic constants, k_i, determine the flux of each complex compound that will be transformed into labile substrates (Ginovart et al., 2005; Gras et al., 2010b).
- Aeration: input flow of oxygen and output flow of carbon dioxide (Ginovart et al., 2005).
- Adsorption and desorption of ammonia (Gras et al., 2010b).

Diffusion of the soluble organic labile substrates and mineral compounds in the medium is modelled according to discrete Fick's law (Ginovart et al., 2005; Prats et al., 2010).

4.6.2 Modelling The Microorganisms

The microorganisms modelled in INDISIM-SOM, as well as the microbial parameters related to their biology and activities have been described in great detail by Ginovart et al. (2005) and Gras et al. (2011). Among all the individual actions or rules of behavior modelled, those that differ the most among INDISIM submodels (Ginovart, López & Valls, 2002; Ginovart et al., 2011) are uptake, metabolism and lysis. They are also the most relevant microbial activities for the soil system under study. In order to use the simulator from the website and to focus on the contents of this description for an appropriate understanding of the variables and parameters involved, only some references to metabolism, death and lysis are detailed here.

After the individual uptake of all substrates (Gras et al., 2011), the microorganism proceeds to metabolize them. The metabolism submodel first considers the cellular maintenance requirements, and after that, if possible, the production of new biomass, with the corresponding release of metabolic or end products. A heterotrophic metabolism is modelled for decomposers, and an autotrophic metabolism for nitrifiers. For cellular maintenance, the heterotrophic individuals use energy substrates following the sequence labile C,

labile N, and own biomass (in the event that non-labile organic substrates are available). The individual energy requirement, m_e, is assumed to be proportional (E^m_i) to the microbial biomass, m, as follows (i = 1 for heterotrophics and i = 2 for nitrifiers): $m_e = E^m_i\, m$. If the individual achievement is sufficient to accomplish its energy requirements, then the microorganism will use the rest of the uptaken substrate for biomass synthesis. For the production of new biomass, the microorganism uses labile C as a C source, and labile N, ammonia or nitrate as an N source. The synthesized biomass keeps the ratio C/N defined for each microbial prototype. The non-metabolized organic substrates that are uptaken are stored in the microorganisms, and can be used at the next time step. The nitrifiers use ammonia as an energy-giving substrate for maintenance and synthesis, while carbon dioxide is used as a C source and ammonia as an N source for biomass production.

Individuals die when they reach a biomass that is below the minimum mass value, known as death probability (d_i), which is 0.001 and 0.004 h^{-1} for heterotrophics and nitrifiers, respectively ($i = 1,2$). When the microorganism dies, its biomass then returns to the media as polymerized compounds, while a fraction, h_3, returns to humic compounds, for the humification process.

5 LEARNING AND TEACHING WITH VIRTUAL EXPERIMENTS FROM THE INDISIM-SOM WEBSITE

The simulator can be useful for practical training in advanced or specialized courses, as support for theoretical lessons in the area of soil science or for modelling in related subjects. If it is used for soil science learning, it is helpful in two ways: as a tool to organize classroom activities based on case studies in which the student can run simulations and obtain output data for analysis, or as a prior study in the design of experiments. This web simulator may also be of use to introduce students to the possibilities of the individual-based modelling methodology, as the microbial model is quite sophisticated and the evolution of the system is dependent on all the individual actions performed by the two microbial prototypes involved. Learners or users can change microbial parameters and test how the soil system reacts, and how the interactions between subpopulations emerge. To run the simulator on the website, one must register and request a username and password to log in. Once logged in, a screen appears displaying a table with the input data that may be modified by the user (Table 1). The values to be assigned to each variable must fall within a specific range, as the simulator does not perform properly with values outside this range.

Parameter description	***Symbol***	***Unit***	***Value***	
Time steps		*hours*	*1800 (1-3000)*	
Soil Organic Carbon	C_{ORG}	*pg/g soil*	$2.175\cdot10^{10}$ $(0\text{-}5\cdot10^{10})$	
Soil Organic Nitrogen	N_{ORG}	*pg/g soil*	$2.175\cdot10^{9}$ $(0\text{-}5\cdot10^{9})$	
Organic N easily hydrolysable	N_{EH}	*pg/g soil*	$1.31\cdot10^{8}$ $(0\text{-}5\cdot10^{8})$	
Ammonium	$N\text{-}N_{NH4}$	*pg/g soil*	$2\cdot10^{7}$ $(0\text{-}5\cdot10^{7})$	
Nitrate	$N\text{-}N_{NO3}$	*pg/g soil*	$3.3\cdot10^{7}$ $(0\text{-}5\cdot10^{7})$	
Partitioning constants				
Fraction of microbial C to organic C	h_0	*adimensional*	*0.015*	
Fraction of labile C	h_1	*adimensional*	*0.065*	
Microbial parameters			*Heterotrophic(i = 1)*	*Nitrifier(i = 2)*
Maintenance energy	E^m_i	$g\ C\ g^{-1}\ C_{MIC}\ h^{-1}$	*0.004 (0.002-0.006)*	*0.008 (0.004-0.01)*
Fraction of Microbial biomass to humified compounds	h_3	*adimensional*	*0.5 (0.0-1.0)*	
Death probability	d_i	h^{-1}	*0.005 (0.0-0.01)*	*0.01 (0.0-0.2)*

Table 1. Default values for running the simulations, and the range of values in which they may be run (in brackets)

Classroom activities were carried out using the INDISIM-SOM simulator with a group of 30 second year students of Biosystems Engineering at the Universitat Politècnica de Catalunya http://www.upc.edu/learning/schools/esab. An initial questionnaire was prepared to assess the students' previous knowledge of some of the aspects dealt with by this simulator, and to be able to compare the

acquisition of further notions and skills at the end of the activities. The responses from the 30 students who completed this initial questionnaire before the use of INDISIM-SOM were collected and subsequently analysed. The questions the students were asked dealt with simple ideas and concepts associated with the composition of SOM, mineralization of SOM, nitrification process in soil, and the pathways and substrates that can be used by microorganisms in the soil, distinguishing between decomposers, which have a heterotrophic metabolism, and nitrifier bacteria, with an autotrophic metabolism. Unexpectedly, the responses related to this body of knowledge were disappointing; no student managed to answer more than the half of these questions correctly. In addition to this set of test questions, some open-ended questions were asked in order to gather more individualized information regarding the level of these students. In response to the question of whether they had previously had the opportunity to work with mathematical or computational models applied to microbial systems, the answer was "No" for 66% of the students. Affirmative answers were related to the possible extension of the use of the NetLogo platform, an environment that had been used the year before in Mathematics (Ginovart et al., 2012). In addition, it was perceived that the application of laws and formulas had not been clearly connected with the possibility of using a model to represent a system as complex as the soil system. From the preliminary information gathered from the initial questionnaire, it was established that these second-year university students of Biosystems Engineering had not yet achieved soil modelling competence or they had not had the opportunity to develop it. This meant that we had a very good occasion to conduct activities involving practice with modelling and simulation in real-life contexts, such as with a soil system, an option that was made possible by INDISIM-SOM.

Teaching material was given to the students to perform the core part of the activity, with some suggestions on the use of the simulator to guide them through the main parts of the computational model. First, the students were asked to carefully read the documentation displayed in the introduction window of the INDISIM_SOM website at https://aneto.upc.es/simulacio2/hoja-portada.html and to list the different elements, processes and parameters considered in its design and formulation. There are significant notions or ideas involved in this model that have a biological meaning. The students were asked to carry out the "demo" simulation, keeping all the default values and observing the outcomes generated by the simulator, and then to write a report with their reflections on the simulated temporal evolutions, as well as the real possibility of achieving this type of results in an experimental trial (in a laboratory or field setting). After that, different virtual experiments were proposed to continue the activity. We suggested investigating the behavior of the simulator at different levels and for different purposes. For instance, one objective could be to check whether the simulator is able to reproduce the C and N mineralization and nitrification processes for soils with different SOMs. To achieve this goal, five virtual soils have been designed, each one of them defined by its organic C content. The other experimental determinations related to C and N considered in the experimental analyses were proportional to this variable in order to prevent interactions attributable to the different sizes of the pools considered in the model, so the relative size between them was kept the same for all soils (Table 2). The evolutions over time of the five virtual soils with different organic C contents and proportional organic N, easily hidrolyzable N, nitrate and ammonia contents were generated on the website.

				Simulations		
pg	***Ratios***	***0.5% C_{ORG}***	***1.25% C_{ORG}***	***2% C_{ORG}***	***2.75% C_{ORG}***	***3.5% C_{ORG}***
Organic Carbon		*$5.0 \cdot 10^{9}$*	*$1.25 \cdot 10^{10}$*	*$2.0 \cdot 10^{10}$*	*$2.75 \cdot 10^{10}$*	*$3.50 \cdot 10^{10}$*
Organic Nitrogen	*C/N=10*	*$5.0 \cdot 10^{8}$*	*$1.\ 25 \cdot 10^{9}$*	*$2.0 \cdot 10^{9}$*	*$2.75 \cdot 10^{9}$*	*$3.5 \cdot 10^{9}$*
Easily Hidrolyzable Nitrogen	*N_{EH}/N_{ORG}=0.066*	*$3.3 \cdot 10^{7}$*	*$8.25 \cdot 10^{7}$*	*$1.32 \cdot 10^{8}$*	*$1.815 \cdot 10^{8}$*	*$2.31 \cdot 10^{8}$*
Ammonia	*N_{NH4}/N_{ORG}=0.010*	*$5.0 \cdot 10^{6}$*	*$1.25 \cdot 10^{7}$*	*$2.0 \cdot 10^{7}$*	*$2.75 \cdot 10^{7}$*	*$3.5 \cdot 10^{7}$*
Nitrate	*N_{NO3}/N_{ORG}=0.020*	*$1.0 \cdot 10^{7}$*	*$2.5 \cdot 10^{7}$*	*$4.0 \cdot 10^{7}$*	*$5.5 \cdot 10^{7}$*	*$7.0 \cdot 10^{7}$*

Table 2. Input soil data for running the simulations

6 SOME SIMULATION RESULTS AND DISCUSSION

The graphical output shown on this website allows the user to visualize how the system's variables change in different scenarios. The output data are generated using the graphical interface of the web simulator, displaying temporal evolutions of a number of state variables as a set of graphs (Gras et al., 2010a). The related output variables shown are classified into two groups. The first shows the number of heterotrophic individuals and nitrifier bacteria, the ratio of microbial C to organic C, the C to N microbial ratio, and the amount of oxygen

in the soil atmosphere (%). These variables are represented in Figure 1. The other group of output graphics show the net production of CO_2 (µg CO_2 g^{-1}), the easily hydrolysable N (µg $N\text{-}N_{EH}$ g^{-1}), mineral N (µg N_{MIN} g^{-1}), ammonium (µg $N\text{-}NH_4$ g^{-1}) and nitrate in the soil solution (µg $N\text{-}NO_3$ g^{-1}). These are represented in Figure 2.

Conducting virtual experiments poses many advantages for teaching and learning, in that it complements experimental assays. One such advantage is the possibility to run all the simulations, the "equivalent" of many experiments that would take much longer to carry out in a laboratory, in a very short time. The introduction to modelling and simulation methodology in a scientific field and in a classroom allows us to develop some the different levels of Bloom's Taxonomy in the cognitive domain and make the learning experience more pleasant and successful. Before or during the use of the INDISIM-SOM simulator, the students should know the foundation of soil system functioning (First level: knowledge). Then from a given scenario suggested by the teacher, they must run the simulation, collect the output data and interpret their meaning (Second level: comprehension) (Figures 1 and 2). If necessary, the following must also be carried out: calculation of other ratios that better explain the results and allow the interpretation of how the interactions emerge from the reliability of individual system components, evaluation of the pattern of output variables, as well as the values produced at the end of the simulation experiments, and the programming of different scenarios and the collection of output data, to determine differences in the behavior of the system (Third level: application) (Figure 3). Eventually, in a more advanced course, working with this kind of model may encourage students to improve or change some parts of the model or to develop new approaches. All of these activities lead to the acquisition of the skills and expertise that correspond to higher levels of education.

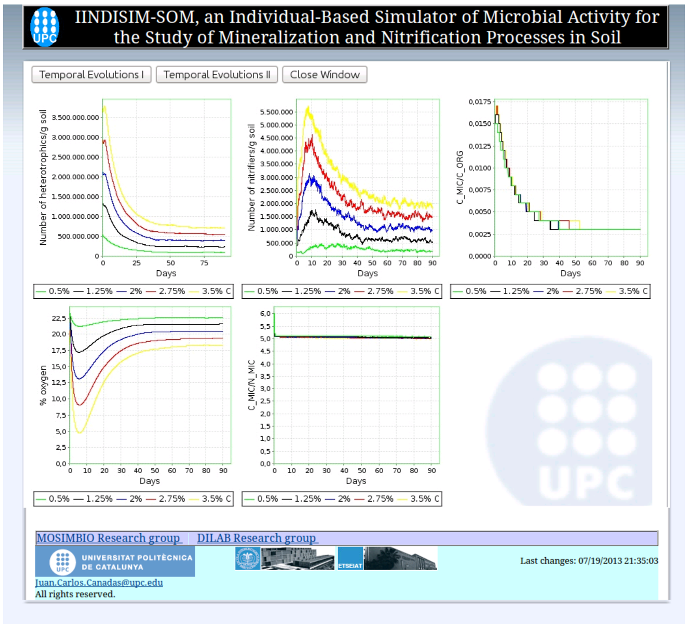

Figure 1. Temporal evolution of microbial variables, for virtual soils with 0.5, 1.25, 2.0, 2.75 and 3.5 % of C. Number of heterotrophics, number of nitrifiers, ratio of microbial C in organic C to oxygen, and C to N ratio of microbial biomass

The results obtained after running the programmed simulations show the temporal evolutions of the variable output that are in accordance with what is expected for the developed model (Figures. 1 and 2). The differences obtained for microbial C are only significant in terms of the maximum reached for each soil, showing higher levels when organic C was also high. However, the differences found at the end of the simulation are much smaller. These results mean that once the initial labile organic C is depleted, only the microbial biomass remains that the soil is able to maintain, which depends upon its humic organic matter and its decay. If students or scientists are motivated to learn more about the system, they can then proceed to extract the net C and N mineralization at the end of the evolution and study the correlation between these variables and the organic C content. They may realize that the net C and N mineralization and the net production of ammonia and nitrate do not demonstrate a linear relationship with the organic C content in the ranges tested, despite the fact that the virtual soil determinations are linear (Figure 3). It is possible to verify

that the nitrification of mineral N is much greater in soils with higher organic C, probably due to the higher N mineralization, enhancing the availability of ammonia. This allows the nitrifiers to be more efficient in the use of , which increases the growth rate (Figure 3).

Most of the answers collected in the part of the activity concerning the different elements of the model and the various outcomes for the set of simulations provided correct or reasonably correct responses. The student realised that although the characteristics or rules that may be assigned to the individuals and the resources in the environment are simple and comprehensible in an isolated way, when we incorporate and integrate everything in a computer code, the complete model attains a considerable degree of complexity. The students indicated that the rules of behavior on which the INDISIM-SOM was based were an approximation of the real situation. Also, the difficulty in obtaining experimental data in this context was evident and extraordinary, so the students were appreciative of the opportunity to manage simulated data.

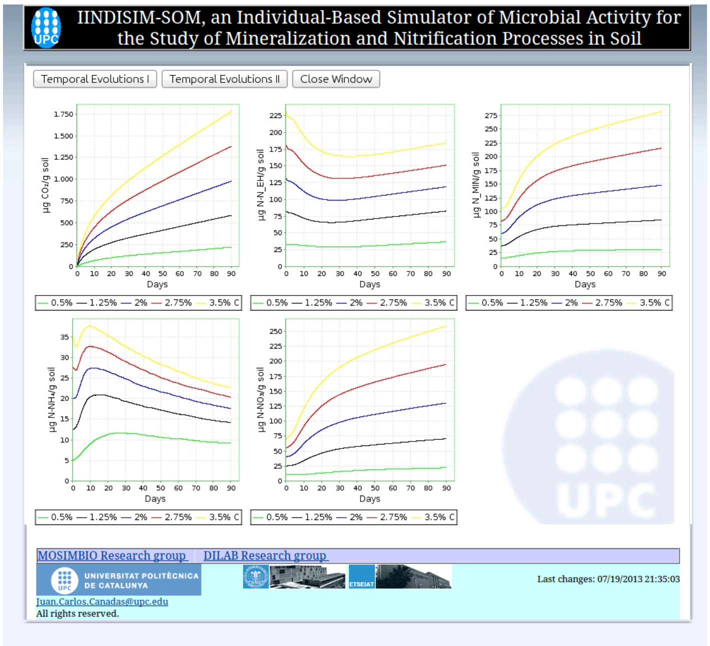

Figure 2. Temporal evolution of C and N mineralization and nitrification variables for virtual soils with, 0.5, 1.25, 2.0, 2.75 and 3.5 % of C. Net production of CO_2, easily hydrolizable N, N_{EH}, total mineral N, ammonia and nitrate

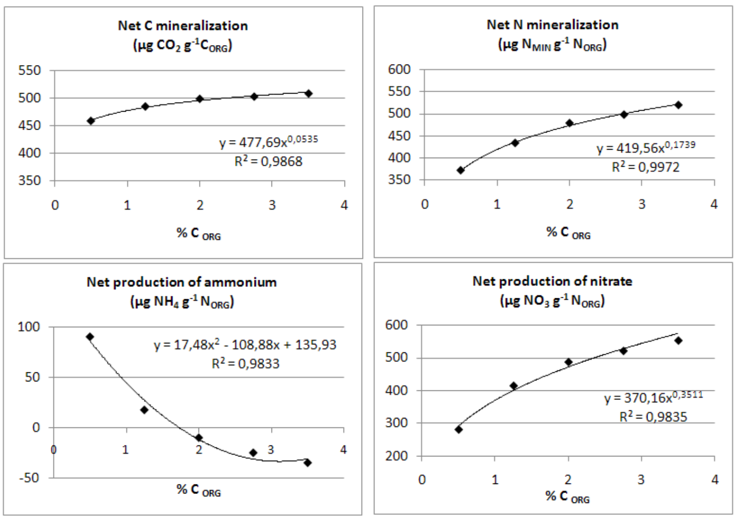

Figure 3. Gross C and N mineralization and net production of ammonia and nitrate at the end of the simulation, in relation to organic C content of the soil

Some of the students' textual comments regarding the use of the simulator INDISIM-SOM are as follows:

- "I considered it to be a very positive experience. It is possible to obtain visual information and it is a way to study the contents in a more dynamic and practical manner. This gives us an idea of the behavior of the system and a better understanding of the interactions taking place in the soil."
- "A very good tool for classroom learning."
- "On one hand it introduces us to a new world, an expanding field with great possibilities for the future. On the other, it also provides a new vision of the traditional concepts explained in class, such as microbiology or soil science. Knowledge does not simply remain on paper, rather it is incorporated in a real, useful context. In this way, the information acquired becomes a tool for future work, and it does not just get stored away in a corner of the brain."
- "By using the simulator, we can see many aspects beforehand, even before conducting a laboratory experiment, which helps reduce the time and cost of the trials."
- "It is interesting to create models and simulators that allow us to simplify what happens in real life, to see things more clearly and understand them better".
- "To better understand and use the simulator, I think that it is necessary to learn more about it and have more time to be able to analyze its complete structure and functioning."
- "I find the simulator more helpful than a written text or an equation."

The compilation and summary of the different answers from the students' reports on this last part of the activity involving the use of different percentages of organic matter, along with their personal opinions about the INDISIM-SOM simulator led us to conclude that this tool has played a significant role in the teaching-learning soil biological processes. We believe that this tool effectively addresses and largely fulfills a very clear need in the classroom.

7 CONCLUSIONS

There are currently very few models that can be used in the limited amount of time available in an academic year for the study of soil or natural science. Furthermore, not all methods or types of models are applicable to all problems. Each model developed, implemented, parameterized, calibrated and corroborated gives an idea of how the system under study functions, and this in itself is a great achievement.

IBMs offer a different perspective of modelling from more continuous mathematical modelling methods, while at the same time contributing complementary information for the study of biosystems by undergraduate and graduate students. IBMs present some very attractive characteristics for developing competence in modelling. They are intuitive and introduce many of the aspects that need to be considered in any modelling process of a living system, many of which are neglected in the majority of analytical models: variability in individuals, local interactions, complete life cycles, and in particular, the adaptation of individual conduct to both internal and external changes in the environment.

In spite of the fact that IBMs have already established a place for themselves in the field of science, these models, as far as we know, have not been included in most academic curricula. IBMs are currently being consolidated in the area of biosystem research, and thus we believe that the moment has come for them to gain ground in education. The ODD protocol for their description and the progressive development of platforms (freely accessible on the Web) are two decisive factors in favor of their introduction in courses.

INDISIM-SOM provides a very good opportunity for experimenting extensively with the implementation and execution of an IBM. We have used this interactive website to provide the option of showing a wide audience how an IBM is able to reproduce the temporal changes of C and N in soils under certain conditions, as well as some of the specific (and interesting) capabilities of this simulator. It is now easier to verify graphically how this simulator works when data that emulate different types of soils or diverse microbial populations are used as input simulation values. At the same time, introducing this simulator to soil scientists, researchers and teachers is a goal in and of itself; since it is accessible on the Internet, interested users can carry out any simulation they like, with little effort.

We are convinced that this work will encourage and facilitate the inclusion of IBMs in academic curricula in general, and in courses on soil science or natural resources in particular. This will contribute to the acceptance of IBMs in the field of computers and education.

ACKNOWLEDGEMENTS

The financial support of the Spanish Government (MICINN, CGL2010-20160) is gratefully acknowledged. We would like to express our most sincere thanks to Dr. Rosa Carbó for giving us the opportunity to carry out the practical activity with the simulator INDISIM-SOM in her classroom.

REFERENCES

Bravo, C., van Joolingen, W.R., & de Jong, T. (2009). Using Co-Lab to build system dynamics models: Student's actions and on line tutorial advice. *Computers & Education,* 53, 243-251. http://dx.doi.org/10.1016/j.compedu.2009.02.005

Faraco, G., & Gabriele, L. (2007). Using LabVIEW for applying mathematical models in representing phenomena. *Computers & Education, 49*, 856-872. http://dx.doi.org/10.1016/j.compedu.2005.11.025

Ginovart, M., López, D., & Valls, J. (2002) INDISIM, an individual based discrete simulation model to study bacterial cultures. *Journal of Theoretical Biology, 214*, 305-319. http://dx.doi.org/10.1006/jtbi.2001.2466

Ginovart, M, Gras, A, & López, D. (2005). Individual-based modelling of microbial activity to study mineralization of C and N and nitrification process in soil. *NonLinear Analysis: Real World Applications,* 6, 773-795. http://dx.doi.org/10.1016/j.nonrwa.2004.12.005

Ginovart, M., Prats, C., Portell, X., & Silbert, M. (2011). Analysis of the effect of inoculum characteristics on the first stages of a growing yeast population in beer fermentations by means of an Individual-based Model. *Journal of Industrial Microbiology and Biotechnology,* 38, 153-165. http://dx.doi.org/10.1007/s10295-010-0840-4

Ginovart, M., Portell, X., Ferrer-Closas, P., & Blanco, M. (2012). Modelos basados en el individuo: una metodologia alternativa y atractiva para el estudio de biosistemas. *Enseñanza de las ciencias,* 30, 93-108.

Gras, A., Cañadas, J.C., & Ginovart, M. (2010a). INDISIM-SOM: an individual-based simulator on a website for experimenting and investigating diverse dynamics of Carbon and Nitrogen in mineral soils. In A. Mendez-Vilas, *Microorganisms in industry and environment. from scientific and industrial research to consumer products* (pp.167-171). World Scientific Publishing Co.

Gras, A., Ginovart, M., Portell, X., & Baveye, P.C. (2010b). Individual-based modelling of carbon and nitrogen dynamics in soils: Parameterization and sensitivity analysis of abiotic components. *Soil Science,* 175, 363-374. http://dx.doi.org/10.1097/SS.0b013e3181eda507

Gras, A., Ginovart, M., Valls, J., & Baveye, P.C. (2011) Individual-based modelling of carbon and nitrogen dynamics in soils: Parameterization and sensitivity analysis of microbial components. *Ecological Modelling,* 222, 1998-2010. http://dx.doi.org/10.1016/j.ecolmodel.2011.03.009

Grimm, V. & Railsback, S.F. (2005). *Individual-based modelling and ecology*. Princeton and Oxford: Princeton University Press.

Grimm, V., Berger, U., Bastiansen, F., Eliassen, S., Ginot, V., Giske, J., et al. (2006). A standard protocol for describing individual-based and agent-based models. *Ecological modelling,* 198, 115-126. http://dx.doi.org/10.1016/j.ecolmodel.2006.04.023

Grimm, V., Berger, U., DeAngelis, D.L., Polhill, J.G., Giske, J., & Railsback, S.F. (2010). The ODD protocol: A review and first update. *Ecological Modelling,* 221, 2760-2768. http://dx.doi.org/10.1016/j.ecolmodel.2010.08.019

Hellweger, F.L., & Bucci, V. (2009). A bunch of tiny individuals-Individual-based modeling for microbes. *Ecological Modelling, 220*, 8-22. http://dx.doi.org/10.1016/j.ecolmodel.2008.09.004

Jacobson, A.R., Militello, R., & Baveye, P.C. (2009). Development of computer-assisted virtual fields trips to support multidisciplinary learning. *Computers & Education,* 52, 571-580. http://dx.doi.org/10.1016/j.compedu.2008.11.007

Justi, R. (2006). La enseñanza de ciencias basada en la elaboración de modelos. *Enseñanza de las Ciencias,* 24, 173-184.

Levy, S.T., & Wilensky, U. (2011). Mining students' inquiry actions for understanding of complex systems. *Computers & Education,* 56, 556-573. http://dx.doi.org/10.1016/j.compedu.2010.09.015

Manzoni, S, & Porporato, A. (2009). Soil carbon and nitrogen mineralization: Theory and models across scales. *Soil Biology & Biochemistry,* 41, 1355-1379. http://dx.doi.org/10.1016/j.soilbio.2009.02.031

McLane, A.J., Semeniuk, C., McDermid, G.J., & Marceau, D.J. (2011). The role of agent-based models in wildlife ecology and management. *Ecological Modelling,* 222, 1544-1556. http://dx.doi.org/10.1016/j.ecolmodel.2011.01.020

Murray, J.D. (1990). *Mathematical biology*. Berlin Heidelberg: Springer-Verlag.

Peck, S.L. (2004). Simulation as experiment: a philosophical reassessment for biological modelling. *Trends in Ecology and Evolution,* 19, 530-534. http://dx.doi.org/10.1016/j.tree.2004.07.019

Prats, C., Ferrer, J., Gras, A., & Ginovart, M. (2010). Individual-based modelling and simulation of microbial processes: yeast fermentation and multi-species composting. *Mathematical and Computer Modelling of Dynamical Systems,* 16, 489-510. http://dx.doi.org/10.1080/13873954.2010.481809

Railsback, S.F. & Grimm, V. (2011). *Agent-Based and Individual-Based Modeling: A Practical Introduction*. Princeton and Oxford: Princeton University Press.

Scheffer, M., Baveco, J.M., DeAngelis, D.L., Rose, K.A., & van Nes, E.H. (1995). Super-individuals a simple solution for modelling large populations on an individual basis. *Ecological Modelling,* 80, 161-170. http://dx.doi.org/10.1016/0304-3800(94)00055-M

Silva, R.G., Jorgensen E. E., Holub S. M., & Gonsoulin M. E. (2005) Relationships between culturable soil microbial populations and gross nitrogen transformation processes in a clay loam soil across ecosystems. Nutrient Cycling in Agroecosystems. New York, NY: Formerly Kluwer Academic Publishers. *Springer Science and Business Media B.V.,* 71, 259-270.

Thompson, K., & Reimann, P. (2010). Patterns of use of an agent-based model and a system dynamics model: The application of patterns of use and the impacts on learning outcomes. *Computers & Education,* 54, 392-403. http://dx.doi.org/10.1016/j.compedu.2009.08.020

Wilensky, U. & Reisman, K. (2006). Thinking Like a Wolf, a Sheep, or a Firefly: Learning Biology Through Constructing and Testing Computational Theories - An Embodied Modeling Approach. *Cognition and Instruction,* 24, 171-209. http://dx.doi.org/10.1207/s1532690xci2402_1

Citation: Gras, A., Cañadas, J.C. & Ginovart M. (2013). A free accessible individual-based simulator enabling virtual experiments on soil organic matter processes in classroom. *Journal of Technology and Science Education (JOTSE), 3(2), 73-88.* http://dx.doi.org/10.3926/jotse.72

On-line ISSN: 2013-6374 – Print ISSN: 2014-5349 – DL: B-2000-2012

AUTHORS BIOGRAPHY

Anna Gras

She has a degree in Agronomic Engineer at the UdL and the corresponding PhD. She is professor at the UPC in Agri-food engineering and Biotechnology department. Her current research interests are about the development of Individual based models applied to microbiological systems such as soil among others.

Juan Carlos Cañadas

He obtained the Ph.D. degree at the Technical University of Catalonia (UPC).He is currently a Professor in the Department of Physics and Nuclear Engineering, where he is also a member of the research Group of Dielectric Materials. His current research interests include the electrical properties of dielectric materials (relaxations, space charge distribution, the glass transition) and the electrical characterization of insulating materials.

Marta Ginovart

She studied Mathematics at the Universitat Autònoma de Barcelona and she achieved her PhD in Simulation in Sciences at the Universitat Politècnica de Catalunya (Barcelona, Spain). She is working in the Department of Applied Mathematics of this university with the position of Associate Professor. Her research interests include discrete modelling and simulation of biological systems, mainly agent-based models, applied statistics and mathematics education.

Published by OmniaScience (www.omniascience.com)

Journal of Technology and Science Education, 2013 (www.jotse.org)